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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 28	CA/CAPLUS patent coverage enhanced
NEWS	3	JUL 28	EPFULL enhanced with additional legal status information from the EPOLINE Register
NEWS	4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	5	JUL 28	STN Viewer performance improved
NEWS	6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	7	AUG 13	CA/CAPLUS enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	9	AUG 15	CAPLUS currency for Korean patents enhanced
NEWS	10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	12	SEP 25	CA/CAPLUS current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS	13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and Korean patents enhanced
NEWS	14	SEP 29	IFICLS enhanced with new super search field
NEWS	15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS	16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS	17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS	18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS	19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.			

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NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

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* * * * * STN Columbus * * * * *

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	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red Folder\10524345\577.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 00:33:59 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2 TO 124

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 00:34:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 37 TO ITERATE

100.0% PROCESSED 37 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L3 14 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	181.12	181.33

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18

FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 3 L3

=> s l4 and lim, z?/au

41 LIM, Z?/AU

L5 1 L4 AND LIM, Z?/AU

=> d l5, ibib abs hitstr, 1

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:395258 HCAPLUS

DOCUMENT NUMBER: 142:446921

TITLE: A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors

INVENTOR(S): Lim, Ze-Yi; Wang, Haishan; Zhou, Yan

PATENT ASSIGNEE(S): Sbio Pte. Ltd., Singapore

SOURCE: PCT Int. Appl., 145 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

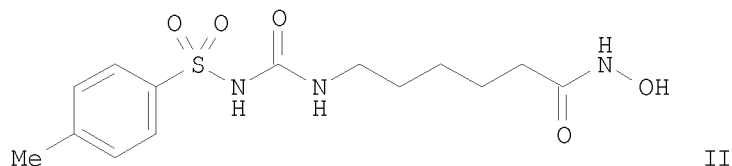
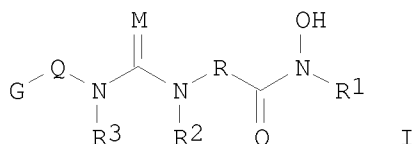
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005040101	A1	20050506	WO 2004-SG353	20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004284030	A1	20050506	AU 2004-284030	20041026
CA 2543570	A1	20050506	CA 2004-2543570	20041026
EP 1685094	A1	20060802	EP 2004-775672	20041026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007509930	T	20070419	JP 2006-537946	20041026
MX 2006PA04735	A	20061214	MX 2006-PA4735	20060427
US 20080070954	A1	20080320	US 2007-577462	20070927
PRIORITY APPLN. INFO.:			US 2003-514013P	P 20031027
			WO 2004-SG353	W 20041026
OTHER SOURCE(S):			CASREACT 142:446921; MARPAT 142:446921	
GI				

Updated Search

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AB The invention relates to a preparation of acylurea- and sulfonylurea-connected hydroxamates of formula I [wherein: R is a linking moiety; R1 is H, alkyl, or acyl; M is O, S, NH, NOH, or N(alkyl), etc.; R2 and R3 are independently selected from H, halogen, alkyl, alk(en/yn)yl, or heteroalkyl, etc.; Q is SO2, C(O), or C(S); G is (cyclo)alkyl, (hetero)aryl, or arylalkyl, etc.], useful as HDAC inhibitors. For instance, hexanoic acid derivative II [IC50 (μM): HDAC1 - >100, HDAC8 - 0.79] was prepared from Me 6-aminohexanoate hydrochloride and phenylsulfonyl isocyanate with a yield of 58%.

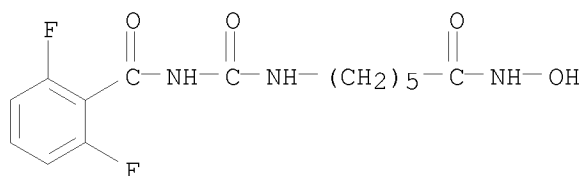
IT 1044042-90-1 1044043-10-8

RL: PRPH (Prophetic)

(A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors)

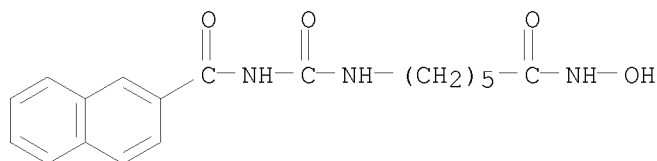
RN 1044042-90-1 HCAPLUS

CN Benzamide, 2,6-difluoro-N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]-
(CA INDEX NAME)



RN 1044043-10-8 HCAPLUS

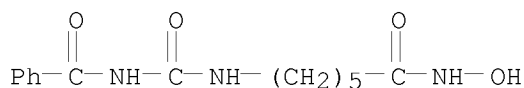
CN 2-Naphthalenecarboxamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]-
(CA INDEX NAME)



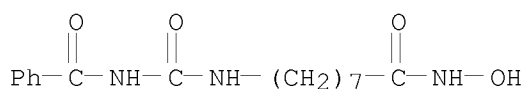
Updated Search

stn

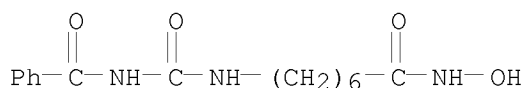
IT 851365-34-9P 851365-36-1P 851365-37-2P
851365-41-8P 851365-43-0P 851365-45-2P
851365-46-3P 851365-48-5P 851365-49-6P
851365-50-9P 851365-70-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of acylurea- and sulfonylurea-connected hydroxamates useful as
HDAC enzyme inhibitors)
RN 851365-34-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX
NAME)



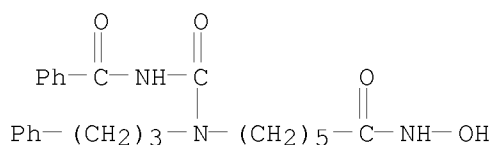
RN 851365-36-1 HCAPLUS
CN Benzamide, N-[[[8-(hydroxyamino)-8-oxooctyl]amino]carbonyl]- (CA INDEX
NAME)



RN 851365-37-2 HCAPLUS
CN Benzamide, N-[[[7-(hydroxyamino)-7-oxoheptyl]amino]carbonyl]- (CA INDEX
NAME)



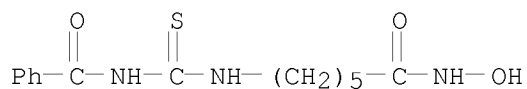
RN 851365-41-8 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](3-
phenylpropyl)amino]carbonyl]- (CA INDEX NAME)



RN 851365-43-0 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]thioxomethyl]- (CA
INDEX NAME)

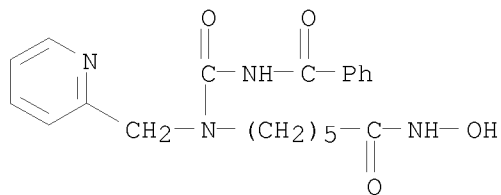
Updated Search

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RN 851365-45-2 HCAPLUS

CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](2-pyridinylmethyl)amino]carbonyl]- (CA INDEX NAME)



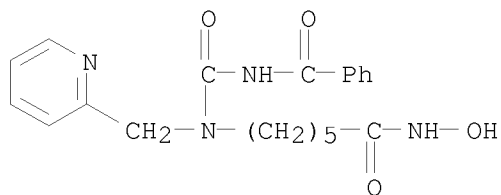
RN 851365-46-3 HCAPLUS

CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](2-pyridinylmethyl)amino]carbonyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 851365-45-2

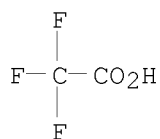
CMF C20 H24 N4 O4



CM 2

CRN 76-05-1

CMF C2 H F3 O2

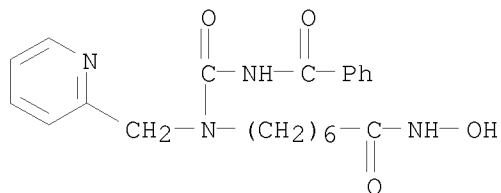


RN 851365-48-5 HCAPLUS

CN Benzamide, N-[[[7-(hydroxyamino)-7-oxoheptyl](2-pyridinylmethyl)amino]carbonyl]- (CA INDEX NAME)

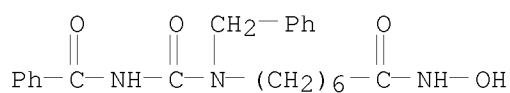
Updated Search

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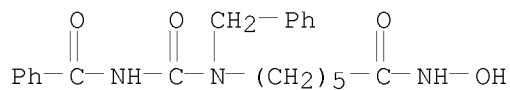
RN 851365-49-6 HCAPLUS

CN Benzamide, N-[[[7-(hydroxyamino)-7-oxoheptyl](phenylmethyl)amino]carbonyl]-
(CA INDEX NAME)



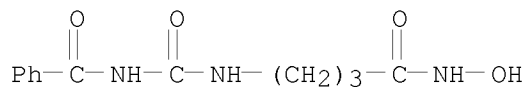
RN 851365-50-9 HCAPLUS

CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](phenylmethyl)amino]carbonyl]-
(CA INDEX NAME)



RN 851365-70-3 HCAPLUS

CN Benzamide, N-[[[4-(hydroxyamino)-4-oxobutyl]amino]carbonyl]- (CA INDEX
NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3

Updated Search

stn

L5 1 S L4 AND LIM, Z?/AU

=> s l4 not l5

L6 2 L4 NOT L5

=> s l6 and wang, h?/au

51308 WANG, H?/AU

L7 0 L6 AND WANG, H?/AU

=> s l6 and zhou, y?/au

21640 ZHOU, Y?/AU

L8 0 L6 AND ZHOU, Y?/AU

=> d l6, ibib abs hitstr, 1-2

L6 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1447760 HCAPLUS

DOCUMENT NUMBER: 148:85678

TITLE: Solid oral dosage form containing deacetylase inhibitor and an enhancer

INVENTOR(S): Leonard, Thomas W.; O'Toole, Edel; Feeney, Orlagh

PATENT ASSIGNEE(S): Merrion Research II Limited, Ire.

SOURCE: U.S. Pat. Appl. Publ., 38pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 20070292512	A1	20071220	US 2007-761233	20070611
WO 2007146234	A2	20071221	WO 2007-US13693	20070611
WO 2007146234	A3	20080228		
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RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

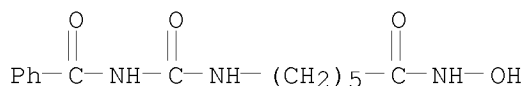
PRIORITY APPLN. INFO.: US 2006-812523P P 20060609

AB The invention relates to a pharmaceutical composition, particularly oral dosage forms, comprising a DAC inhibitor in combination with an enhancer to promote absorption of the DAC inhibitor at the GIT cell lining. The enhancer is a medium-chain fatty acid or derivative thereof having a carbon chain length of 6-20 carbon atoms. In certain embodiments, the solid oral dosage form is a controlled-release dosage form such as a delayed-release dosage form. Thus, a sustained-release tablet was prepared containing sodium caprylate 65.7%, heparin 13.3%, silica dioxide 0.5%, magnesium stearate 0.5%, and mannitol 20.0%.

Updated Search

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IT 851365-34-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(solid oral dosage form containing deacetylase inhibitor and an enhancer)
RN 851365-34-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX NAME)



L6 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:206787 HCAPLUS

DOCUMENT NUMBER: 146:287512

TITLE: Development and validation of high-performance liquid chromatography-tandem mass spectrometry assay for 6-(3-benzoyl-ureido)-hexanoic acid hydroxyamide, a novel HDAC inhibitor, in mouse plasma for pharmacokinetic studies

AUTHOR(S): Yeo, Pauline; Xin, Liu; Goh, Evelyn; New, Lee Sun; Zeng, Peizi; Wu, Xiaofeng; Venkatesh, P.; Kantharaj, Ethirajulu

CORPORATE SOURCE: Department of Pharmacokinetics and Drug Metabolism, SBIO Pte Ltd, Singapore, 117528, Singapore

SOURCE: Biomedical Chromatography (2007), 21(2), 184-189

CODEN: BICHE2; ISSN: 0269-3879

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A liquid chromatog./tandem mass spectrometric method for the quantification of 6-(3-benzoyl-ureido)-hexanoic acid hydroxyamide (EX-2), a novel histone deacetylase (HDAC) inhibitor, in mouse plasma was developed to support inhouse pharmacokinetic (PK) studies in the lead optimization stage. In order to determine the PK parameters for EX-2 in comparison to other HDAC inhibitors such as Suberoylanilide hydroxamic acid (SAHA), PXD-101, and LBH-589, which are currently in different stages of clin. trials, research-grade bio-anal. method validations were carried out for EX-2 and these reference HDAC inhibitors, which were synthesized by inhouse medicinal chemists. The components of validation consisted of specificity, extraction efficiency, signal-response of calibration stds., lower limit of quantification, autosampler stability, and accuracy and precision of quality control samples. The validated LC/MS/MS methods were accurate and precise. The calibration curve ranged from 1 to 1600 ng/mL for all the analytes. The methods developed were used to quantify EX-2 and other HDAC inhibitors in mouse plasma obtained from pharmacokinetic studies. The results suggest that EX-2 has better PK parameters compared with the reference drugs and is a promising drug development candidate.

IT 851365-34-9, EX 2

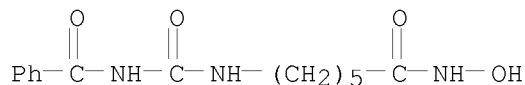
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)

(development and validation of HPLC-tandem mass spectrometry assay for (benzoylureido)hexanoic acid hydroxyamide in mouse plasma for pharmacokinetic studies)

Updated Search

stn

RN 851365-34-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX
NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	19.04	200.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.40	-2.40

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/CAPLUS. To learn more about the options available for transferring saved search queries and answer sets to CA/CAPLUS, contact your STN Service Center.

=> d his

Updated Search

stn

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3

L5 1 S L4 AND LIM, Z?/AU

L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

=> s l3

L9 0 L3

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	200.83
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.40

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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red Folder\10524345\sdfaeat.str

Updated Search

stn

L10 STRUCTURE UPLOADED

=> s l10

SAMPLE SEARCH INITIATED 00:38:12 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 337 TO ITERATE

100.0% PROCESSED 337 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

 BATCH **COMPLETE**

PROJECTED ITERATIONS: 5639 TO 7841

PROJECTED ANSWERS: 3 TO 163

L11 3 SEA SSS SAM L10

=> s l10 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 00:38:16 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6846 TO ITERATE

100.0% PROCESSED 6846 ITERATIONS

66 ANSWERS

SEARCH TIME: 00.00.01

L12 66 SEA SSS FUL L10

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3

L5 1 S L4 AND LIM, Z?/AU

L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

=> s l12 not l3

L13 66 L12 NOT L3

=> file hcaplus

Updated Search

stn

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	180.66	381.49
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.40

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l13

L14 1 L13

=> d l14, ibib abs fhitr, 1

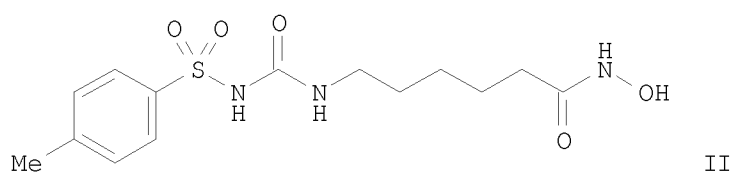
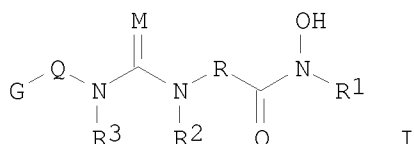
L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:395258 HCAPLUS
DOCUMENT NUMBER: 142:446921
TITLE: A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors
INVENTOR(S): Lim, Ze-Yi; Wang, Haishan; Zhou, Yan
PATENT ASSIGNEE(S): Sbio Pte. Ltd., Singapore
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

Updated Search

stn

WO 2005040101	A1	20050506	WO 2004-SG353	20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004284030	A1	20050506	AU 2004-284030	20041026
CA 2543570	A1	20050506	CA 2004-2543570	20041026
EP 1685094	A1	20060802	EP 2004-775672	20041026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007509930	T	20070419	JP 2006-537946	20041026
MX 2006PA04735	A	20061214	MX 2006-PA4735	20060427
US 20080070954	A1	20080320	US 2007-577462	20070927
PRIORITY APPLN. INFO.:			US 2003-514013P	P 20031027
			WO 2004-SG353	W 20041026
OTHER SOURCE(S): CASREACT 142:446921; MARPAT 142:446921				
GI				



AB The invention relates to a preparation of acylurea- and sulfonylurea-connected hydroxamates of formula I [wherein: R is a linking moiety; R1 is H, alkyl, or acyl; M is O, S, NH, NOH, or N(alkyl), etc.; R2 and R3 are independently selected from H, halogen, alkyl, alk(en/yn)yl, or heteroalkyl, etc.; Q is SO2, C(O), or C(S); G is (cyclo)alkyl, (hetero)aryl, or arylalkyl, etc.], useful as HDAC inhibitors. For instance, hexanoic acid derivative II [IC50 (μM): HDAC1 - >100, HDAC8 - 0.79] was prepared from Me 6-aminohexanoate hydrochloride and phenylsulfonyl isocyanate with a yield of 58%.

IT 1044042-89-8

stn

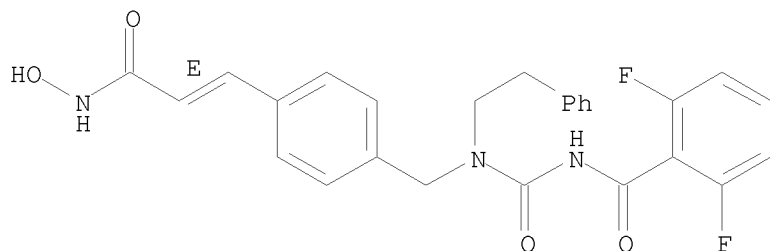
RL: PRPH (Prophetic)

(A preparation of acylurea- and sulfonylurea-connected hydroxamates,
useful as histone deacetylase (HDAC) inhibitors)

RN 1044042-89-8 HCAPLUS

CN Benzamide, 2,6-difluoro-N-[[[4-[(1E)-3-(hydroxyamino)-3-oxo-1-propen-1-yl]phenyl]methyl](2-phenylethyl)amino]carbonyl]- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.14

389.63

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.80

-3.20

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

Updated Search

stn

- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/Caplus. To learn more about the options available for transferring saved search queries and answer sets to CA/Caplus, contact your STN Service Center.

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

=> s l13

L15 0 L13

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	390.09
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-3.20

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

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Updated Search

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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red Folder\10524345\awerat.str

L16 STRUCTURE UPLOADED

=> s l16

SAMPLE SEARCH INITIATED 00:41:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 337 TO ITERATE

100.0% PROCESSED 337 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 5639 TO 7841
PROJECTED ANSWERS: 3 TO 163

L17 3 SEA SSS SAM L16

=> s l16 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED - 6851 TO ITERATE

100.0% PROCESSED 6851 ITERATIONS 69 ANSWERS
SEARCH TIME: 00.00.01

L18 69 SEA SSS FUL L16

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

Updated Search

stn

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL

=> s l18 not l3

L19 69 L18 NOT L3

=> s l19 not l13

L20 3 L19 NOT L13

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-3.20

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 120

L21 1 L20

=> d 121, ibib abs fhitstr, 1

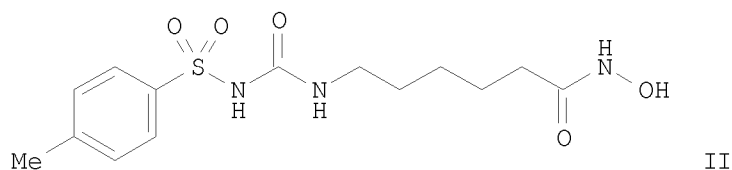
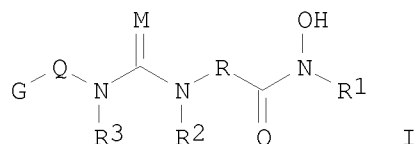
L21 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:395258 HCAPLUS
DOCUMENT NUMBER: 142:446921
TITLE: A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors
INVENTOR(S): Lim, Ze-Yi; Wang, Haishan; Zhou, Yan
PATENT ASSIGNEE(S): Sbio Pte. Ltd., Singapore
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005040101	A1	20050506	WO 2004-SG353	20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004284030	A1	20050506	AU 2004-284030	20041026
CA 2543570	A1	20050506	CA 2004-2543570	20041026
EP 1685094	A1	20060802	EP 2004-775672	20041026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				

Updated Search

stn

JP 2007509930	T	20070419	JP 2006-537946	20041026
MX 2006PA04735	A	20061214	MX 2006-PA4735	20060427
US 20080070954	A1	20080320	US 2007-577462	20070927
PRIORITY APPLN. INFO.:			US 2003-514013P	P 20031027
			WO 2004-SG353	W 20041026
OTHER SOURCE(S):		CASREACT 142:446921; MARPAT 142:446921		
GI				



AB The invention relates to a preparation of acylurea- and sulfonylurea-connected hydroxamates of formula I [wherein: R is a linking moiety; R1 is H, alkyl, or acyl; M is O, S, NH, NOH, or N(alkyl), etc.; R2 and R3 are independently selected from H, halogen, alkyl, alk(en/yn)yl, or heteroalkyl, etc.; Q is SO2, C(O), or C(S); G is (cyclo)alkyl, (hetero)aryl, or arylalkyl, etc.], useful as HDAC inhibitors. For instance, hexanoic acid derivative II [IC50 (μM): HDAC1 - >100, HDAC8 - 0.79] was prepared from Me 6-aminohexanoate hydrochloride and phenylsulfonyl isocyanate with a yield of 58%.

IT 1044042-87-6

RL: PRPH (Prophetic)

(A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors)

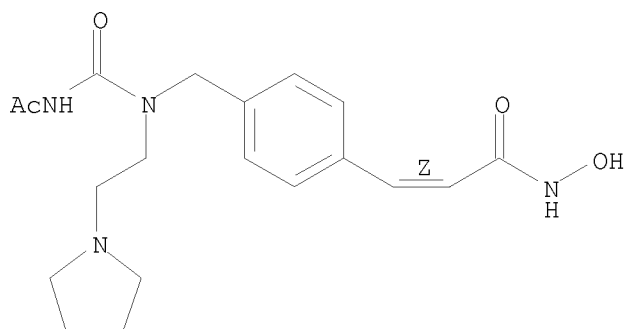
RN 1044042-87-6 HCAPLUS

CN 2-Propenamide, 3-[4-[[[(acetylamino)carbonyl][2-(1-pyrrolidinyl)ethyl]amino]methyl]phenyl]-N-hydroxy-, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

Updated Search

stn



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
8.14	577.97

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.80	-4.00

CA SUBSCRIBER PRICE

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/Caplus. To learn more about the options available for

Updated Search

stn

transferring saved search queries and answer sets to CA/CAPLUS,
contact your STN Service Center.

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

=> s 120

L22 0 L20

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	578.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION

Updated Search

stn

CA SUBSCRIBER PRICE 0.00 -4.00

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\qqtqt.str

L23 STRUCTURE UPLOADED

=> s l23

SAMPLE SEARCH INITIATED 00:44:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 337 TO ITERATE

100.0% PROCESSED 337 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5639 TO 7841
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

=> s l23 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:44:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6851 TO ITERATE

100.0% PROCESSED 6851 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.01

Updated Search

stn

L25 18 SEA SSS FUL L23

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3

L5 1 S L4 AND LIM, Z?/AU

L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED

L17 3 S L16

L18 69 S L16 FULL

L19 69 S L18 NOT L3

L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008

L23 STRUCTURE UPLOADED

L24 0 S L23

L25 18 S L23 FULL

=> s l25 not l13

L26 18 L25 NOT L13

=> s l25 not l3

L27 18 L25 NOT L3

Updated Search

stn

=> s 127 not 118
L28 18 L27 NOT L18

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	180.20	758.63
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.00

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 128
L29 1 L28

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5

Updated Search

stn

L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23 STRUCTURE UPLOADED
L24 0 S L23
L25 18 S L23 FULL
L26 18 S L25 NOT L13
L27 18 S L25 NOT L3
L28 18 S L27 NOT L18

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29 1 S L28

=> s l29 not l21
L30 0 L29 NOT L21

=> file reg		
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	ENTRY	SESSION
FULL ESTIMATED COST	2.69	761.32
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-4.00

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Updated Search

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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

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Folder\10524345\fdafagt.str

L31 STRUCTURE UPLOADED

=> s l31

SAMPLE SEARCH INITIATED 00:47:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 65 TO ITERATE

100.0% PROCESSED 65 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 817 TO 1783
PROJECTED ANSWERS: 1 TO 80

L32 1 SEA SSS SAM L31

=> s l31 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:47:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1581 TO ITERATE

100.0% PROCESSED 1581 ITERATIONS 23 ANSWERS
SEARCH TIME: 00.00.01

L33 23 SEA SSS FUL L31

=> d his

Updated Search

stn

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

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L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

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L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

L22 0 S L20

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L23 STRUCTURE UPLOADED
L24 0 S L23
L25 18 S L23 FULL
L26 18 S L25 NOT L13
L27 18 S L25 NOT L3
L28 18 S L27 NOT L18

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008

L29 1 S L28
L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008

L31 STRUCTURE UPLOADED

Updated Search

stn

L32 1 S L31
L33 23 S L31 FULL

=> s l33 not l13
L34 23 L33 NOT L13

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	179.74	941.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.00

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l34
L35 12 L34

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

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L4 3 S L3

Updated Search

stn

L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
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L10 STRUCTURE UPLOADED
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FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
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L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
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FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23 STRUCTURE UPLOADED
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L25 18 S L23 FULL
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L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31 STRUCTURE UPLOADED
L32 1 S L31
L33 23 S L31 FULL
L34 23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
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L36 11 L35 NOT L14

Updated Search

stn

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41 LIM, Z?/AU
L38 0 L37 AND LIM, Z?/AU

=> s 137 and wang, h?/au
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L39 0 L37 AND WANG, H?/AU

=> s 137 and zhou, y?/au
21640 ZHOU, Y?/AU
L40 0 L37 AND ZHOU, Y?/AU

=> d 137, ibib abs hitstr, 1-9

L37 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:411563 HCAPLUS
DOCUMENT NUMBER: 140:391128
TITLE: Preparation of β -aminohydroxamic acids as peptide
deformylase (PDF) inhibitors and their medical use
INVENTOR(S): Takayama, Wataru; Shirasaki, Masahisa; Inoue, Atsushi
PATENT ASSIGNEE(S): Senju Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2004143053	A	20040520	JP 2002-307534	20021022
PRIORITY APPLN. INFO.:			JP 2002-307534	20021022

OTHER SOURCE(S): MARPAT 140:391128

AB R2LG1NHCHR1CH2CONHOH [R1 = C1-5 linear or branched alkyl; R2 =
(un)substituted aromatic hydrocarbonyl, (un)substituted heterocyclyl; G1 = CO,
SO2; L = G2NH, (CH2)n, CONR4CHR3, etc.; G2 = CO, SO2, bond; n = 0, 1; R3,
R4 = H, C4-6 alkyl, R3R4 may be bonded to form C3-7 alkylene] or their
salts, useful for inhibition of drug-resistant bacteria, are prepared Thus,
amidation of (3S)-3-aminoheptanoic acid benzyloxyamide HCl salt with
2-naphthoyl chloride and hydrogenation of the product gave
(1S)-naphthalene-2-carboxylic acid
[1-(hydroxycarbamoylmethyl)pentyl]amide, which inhibited Ni-PDF from
Escherichia coli with IC50 value of 4.656 μ M.

IT 688002-83-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of β -aminohydroxamic acids as peptide deformylase
inhibitors and antibacterial agents)

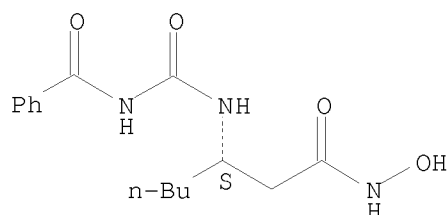
RN 688002-83-7 HCAPLUS

CN Benzamide, N-[[[(1S)-1-[2-(hydroxyamino)-2-oxoethyl]pentyl]amino]carbonyl]-
(CA INDEX NAME)

Updated Search

stn

Absolute stereochemistry.



L37 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:381037 HCAPLUS

DOCUMENT NUMBER: 135:133815

TITLE: Protease Inhibitors: Synthesis of a Series of Bacterial Collagenase Inhibitors of the Sulfonyl Amino Acyl Hydroxamate Type

AUTHOR(S): Clare, Brian W.; Scozzafava, Andrea; Supuran, Claudiu T.

CORPORATE SOURCE: Department of Chemistry, The University of Western Australia, 6009, Australia

SOURCE: Journal of Medicinal Chemistry (2001), 44(13), 2253-2258

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:133815

AB A series of sulfonyl amino acyl hydroxamates incorporating alkyl/arylsulfonyl-N-2-nitrobenzyl-L-alanine was prepared. Related compds. were obtained by reaction of N-2-nitrobenzyl-L-Ala with aryl isocyanates, arylsulfonyl isocyanates, or benzoyl isothiocyanate, followed by the conversion of the COOH into the CONHOH moiety. The new compds. were assayed as inhibitors of the Clostridium histolyticum collagenase (ChC), a bacterial protease involved in the degradation of extracellular matrix. Many of the obtained hydroxamates proved to be effective bacterial collagenase inhibitors, the main contributor to activity being the substitution pattern at the sulfonamido moiety. The best ChC inhibitors were those containing pentafluorophenylsulfonyl and 3- and 4-protected-aminophenylsulfonyl P1' groups among others, with affinities in the low nanomolar range. This study also proves that the 2-nitrobenzyl- moiety, similarly to the 4-nitrobenzyl one previously investigated is an efficient P2' anchoring moiety for obtaining potent bacterial collagenase inhibitors.

IT 351527-61-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of a series of bacterial collagenase inhibitors of the sulfonyl amino acyl hydroxamate type)

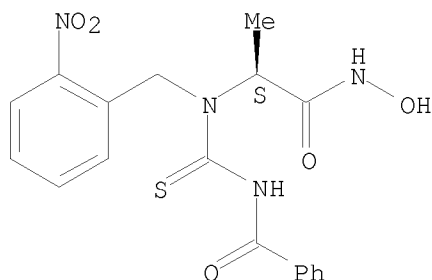
RN 351527-61-2 HCAPLUS

CN Benzamide, N-[[[(1S)-2-(hydroxyamino)-1-methyl-2-oxoethyl]][(2-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)

Updated Search

stn

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:453771 HCAPLUS

DOCUMENT NUMBER: 133:234316

TITLE: Protease inhibitors. Part 12. Synthesis of potent matrix metalloproteinase and bacterial collagenase inhibitors incorporating sulfonlated N-4-nitrobenzyl- β -alanine hydroxamate moieties
AUTHOR(S): Scozzafava, A.; Ilies, M. A.; Manole, G.; Supuran, C. T.

CORPORATE SOURCE: Universita degli Studi, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, I-50121, Italy
SOURCE: European Journal of Pharmaceutical Sciences (2000), 11(1), 69-79

CODEN: EPSCED; ISSN: 0928-0987

PUBLISHER: Elsevier Science Ireland Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-4-Nitrobenzyl- β -alanine was reacted with alkyl/arylsulfonyl halides, followed by conversion of the COOH to the CONHOH group. Structurally related compds. were obtained by reaction of N-4-nitrobenzyl- β -alanine with aryl isocyanates, arylsulfonyl isocyanates or benzoyl isothiocyanate, followed by similar conversion of the COOH into the CONHOH moiety. Another subseries of derivs. was prepared from sulfanilyl- or metanilyl-4-nitrobenzyl- β -alanine by reaction with arylsulfonyl isocyanates, followed by the introduction of the hydroxamate moiety. The new compds. were assayed as inhibitors of four matrix metalloproteinases (MMPs), MMP-1, MMP-2, MMP-8 and MMP-9, and of the Clostridium histolyticum collagenase (ChC). Some of the prepared hydroxamate derivs. proved to be very effective collagenase/gelatinase inhibitors, depending on the substitution pattern at the sulfonamido moiety. Substitutions leading to the best inhibitors of MMP-1, a short-pocket enzyme, were those involving pentafluorophenylsulfonyl or 3-trifluoromethyl-phenylsulfonyl at P1' (KI of 3-5 nM). For MMP-2, MMP-8 and MMP-9 (deep-pocket enzymes), the best inhibitors were those containing perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl-, 3- and 4-carboxy-phenylsulfonyl-, arylsulfonylureido- or arylsulfonylureido-sulfanilyl-/metanilyl moieties at P1'. Bulkier groups

Updated Search

stn

in this position, such as 1- and 2-naphthyl-, substituted-naphthyl or quinoline-8-yl- moieties, among others, led to less effective MMP/ChC inhibitors. The best ChC inhibitors were again those containing pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl P1' groups. This study demonstrates that the 4-nitrobenzyl moiety, investigated here for the first time, is an efficient P2' anchoring moiety, whereas the β -alanyl scaffold can successfully replace the α -amino acyl one, for obtaining potent MMP/ChC inhibitors.

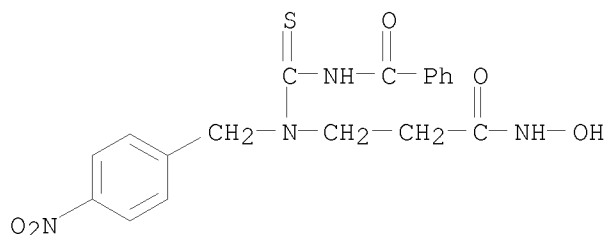
IT 294200-81-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of potent matrix metalloproteinase and bacterial collagenase inhibitors incorporating sulfonylated nitrobenzylalanine hydroxamate moieties)

RN 294200-81-0 HCAPLUS

CN Benzamide, N-[[[3-(hydroxyamino)-3-oxopropyl][(4-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:368315 HCAPLUS

DOCUMENT NUMBER: 133:177439

TITLE: Protease inhibitors: synthesis of L-alanine hydroxamate sulfonylated derivatives as inhibitors of Clostridium histolyticum collagenase

AUTHOR(S): Supuran, Claudiu T.; Briganti, Fabrizio; Mincione, Giovanna; Scozzafava, Andrea

CORPORATE SOURCE: Universita degli Studi, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, I-50121, Italy

SOURCE: Journal of Enzyme Inhibition (2000), 15(2), 111-128
CODEN: ENINEG; ISSN: 8755-5093

PUBLISHER: Harwood Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB L-alanine hydroxamate derivs. were obtained by reaction of alkyl/arylsulfonyl halides with L-alanine, followed by treatment with benzyl chloride, and conversion of the COOH moiety to the CONHOH group with hydroxylamine in the presence of carbodiimides. Other derivs. were obtained by reaction of N-benzyl-alanine with aryl isocyanates, arylsulfonyl isocyanates or benzoyl isothiocyanate, followed by a similar conversion of the COOH to the CONHOH moiety. The obtained compds. were assayed as inhibitors of Clostridium histolyticum collagenase, ChC (EC

Updated Search

stn

3.4.24.3), a zinc enzyme which degrades triple helical collagen. The hydroxamate derivs. were generally 100-500 times more active than the corresponding carboxylates. In the series of synthesized derivs., substitution patterns leading to the most potent ChC inhibitors were those involving perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl-, 3- and 4-protected-aminophenylsulfonyl-, 3- and 4-carboxyphenylsulfonyl-, 3-trifluoromethyl-phenylsulfonyl-, or 1- and 2-naphthylsulfonyl among others. Similarly to the matrix metalloproteinase (MMP) hydroxamate inhibitors, ChC inhibitors of the type reported here must incorporate hydrophobic moieties at the P2' and P3' sites, in order to achieve tight binding to the enzyme.

IT 288266-41-1P

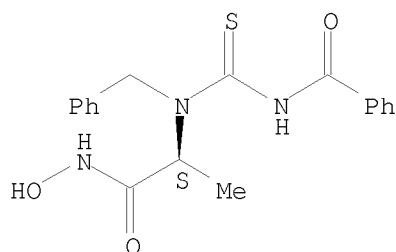
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of L-alanine hydroxamate sulfonylated derivs. as inhibitors of Clostridium histolyticum collagenase)

RN 288266-41-1 HCAPLUS

CN Benzamide, N-[[[(1S)-2-(hydroxyamino)-1-methyl-2-oxoethyl](phenylmethyl)amino]thioxomethyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:261412 HCAPLUS

DOCUMENT NUMBER: 133:53160

TITLE: Protease inhibitors - part 5. Alkyl/arylsulfonyl- and arylsulfonylureido-/arylureido- glycine hydroxamate inhibitors of Clostridium histolyticum collagenase

AUTHOR(S): Scozzafava, Andrea; Supuran, Claudiu T.

CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy

SOURCE: European Journal of Medicinal Chemistry (2000), 35(3), 299-307

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reaction of alkyl/arylsulfonyl halides with glycine afforded a series of derivs. which were first N-benzylated by treatment with benzyl chloride, and then converted to the corresponding hydroxamic acids with

Updated Search

stn

hydroxylamine in the presence of carbodiimide derivs. Other derivs. were obtained by reaction of N-benzyl-glycine with aryl isocyanates, arylsulfonyl isocyanates or benzoyl isothiocyanate, followed by conversion of their COOH group into the CONHOH moiety, as mentioned above. The 90 new compds. reported here were assayed as inhibitors of the *Clostridium histolyticum* collagenase (EC 3.4.24.3), a zinc enzyme which degrades triple helical regions of native collagen. The prepared hydroxamate derivs. were generally 100-500 times more active than the corresponding carboxylates. In the series of synthesized hydroxamates, substitution patterns leading to the best inhibitors were those involving perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-carboxyphenylsulfonyl-, 3-trifluoromethyl-phenylsulfonyl or 1- and 2-naphthyl among others. Thus, it seems that similarly to the matrix metalloproteinase (MMP) hydroxamate inhibitors, *Clostridium histolyticum* collagenase inhibitors should incorporate hydrophobic moieties at the P1' and P2' sites, whereas the α -carbon substituent may be a small and compact moiety (such as H, for the Gly derivs. reported here). Such compds. might lead to the design of collagenase inhibitor-based drugs useful as anti-cancer, anti-arthritis or anti-bacterial agents for the treatment of corneal keratitis.

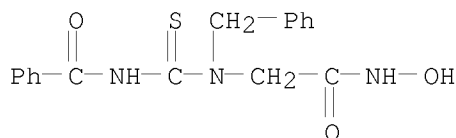
IT 276696-17-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(alkyl/arylsulfonyl- and arylsulfonylureido-/arylureido- glycine hydroxamate inhibitors of *Clostridium histolyticum* collagenase)

RN 276696-17-4 HCAPLUS

CN Benzamide, N-[[[2-(hydroxyamino)-2-oxoethyl](phenylmethyl)amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:222313 HCAPLUS

DOCUMENT NUMBER: 133:26475

TITLE: Protease Inhibitors: Synthesis of Potent Bacterial Collagenase and Matrix Metalloproteinase Inhibitors Incorporating N-4-Nitrobenzylsulfonylglycine Hydroxamate Moieties

AUTHOR(S): Scozzafava, Andrea; Supuran, Claudiu T.

CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy

SOURCE: Journal of Medicinal Chemistry (2000), 43(9), 1858-1865

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

Updated Search

stn

LANGUAGE: English

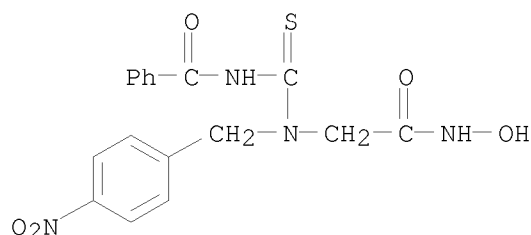
AB A series of compds. was prepared by reaction of alkyl/arylsulfonyl halides with N-4-nitrobenzylglycine, followed by conversion of the COOH to the CONHOH group, with hydroxylamine in the presence of carbodiimides. Other structurally related compds. were obtained by reaction of N-4-nitrobenzylglycine with aryl isocyanates, arylsulfonyl isocyanates, or benzoyl isothiocyanate, followed by the similar conversion of the COOH into the CONHOH moiety. Another subseries of derivs. was prepared from sulfanilyl- or metanilyl-4-nitrobenzylglycine by reaction with arylsulfonyl isocyanates, followed by conversion of the COOH to the hydroxamate moiety. The new compds. were assayed as inhibitors of four matrix metalloproteinases (MMPs), MMP-1, MMP-2, MMP-8, and MMP-9, and of the Clostridium histolyticum collagenase (ChC). Some of the prepared hydroxamate derivs. proved to be very effective collagenase/gelatinase inhibitors, depending on the substitution pattern at the sulfonamido moiety. Substitutions leading to best inhibitors of MMP-1, a short pocket enzyme, were those involving pentafluorophenylsulfonyl or 3-trifluoromethylphenylsulfonyl moieties at P1' (KI's of 3-5 nM). For MMP-2, MMP-8, and MMP-9 (deep-pocket enzymes), best inhibitors were especially those containing long perfluoroalkylsulfonyl and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl, 3- and 4-carboxyphenylsulfonyl, arylsulfonylureido, or arylsulfonylureidosulfanilyl/metanilyl moieties, at P1'. Bulkier groups in this position, such as 1- and 2-naphthyl, substituted-naphthyl, or quinolin-8-yl moieties among others, led to less effective MMP/ChC inhibitors. Best ChC inhibitors were again those containing pentafluorophenylsulfonyl or 3- and 4-protected-aminophenylsulfonyl P1' anchoring groups, suggesting that this protease is also a short-pocket wider-neck one (more similar to MMP-1). This study also proves that the 4-nitrobenzyl moiety is an efficient P2' anchoring moiety and that sulfonylureido, ureido, or carboxythioureido substitutions at P1' are also tolerated for obtaining potent sulfonylated amino acid hydroxamate-like MMP/ChC inhibitors.

IT 273732-17-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis of potent bacterial collagenase and matrix metalloproteinase inhibitors incorporating nitrobenzylsulfonylglycine hydroxamate moieties)

RN 273732-17-5 HCAPLUS

CN Benzamide, N-[[[2-(hydroxyamino)-2-oxoethyl][(4-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

stn

L37 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

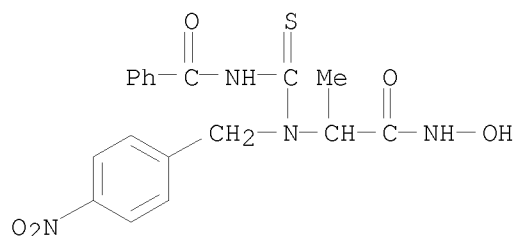
ACCESSION NUMBER: 2000:208763 HCAPLUS
DOCUMENT NUMBER: 132:305057
TITLE: Protease inhibitors: synthesis of Clostridium histolyticum collagenase inhibitors incorporating sulfonyl-L-alanine hydroxamate moieties
AUTHOR(S): Scozzafava, Andrea; Supuran, Claudiu T.
CORPORATE SOURCE: Universita degli Studi, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, 50121, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(5), 499-502
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of hydroxamates was obtained by the reaction of N-(4-nitrobenzyl)-L-alanine with alkyl/arylsulfonyl halides, followed by conversion of the CO₂H group into CONHOH (no data). Structurally related compds. were prepared similarly by using arylsulfonyl isocyanates, aryl isocyanates or arylsulfonyl halides instead of the sulfonyl halides (no data). Many of the new compds. showed nanomolar affinity for the bacterial collagenase isolated from the pathogen Clostridium histolyticum.

IT 265668-57-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Clostridium collagenase inhibitors incorporating sulfonylalanine hydroxamate)

RN 265668-57-3 HCAPLUS

CN Benzamide, N-[[[2-(hydroxyamino)-1-methyl-2-oxoethyl][(4-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:157028 HCAPLUS
DOCUMENT NUMBER: 132:344757
TITLE: Protease inhibitors. Part 8. Synthesis of potent Clostridium histolyticum collagenase inhibitors incorporating sulfonylated L-alanine hydroxamate moieties
AUTHOR(S): Scozzafava, A.; Supuran, C. T.
CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy

Updated Search

stn

SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(3), 637-645
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of hydroxamates was prepared by reaction of alkyl/arylsulfonyl halides with N-2-chlorobenzyl-L-alanine, followed by conversion of the CO₂H moiety to the CONHOH group, with NH₂OH in the presence of carbodiimides. Other structurally related compds. were obtained by reaction of N-2-chlorobenzyl-L-alanine with aryl isocyanates, arylsulfonyl isocyanates, or benzoyl isothiocyanate, followed by the similar conversion of the CO₂H into the CONHOH moiety. The new compds. were assayed as inhibitors of the Clostridium histolyticum collagenase, ChC (EC 3.4.24.3), a bacterial Zn metallo-peptidase which degrades triple helical collagen as well as a large number of synthetic peptides. The prepared hydroxamates proved to be 100-500+ more active collagenase inhibitors than the corresponding carboxylates. Substitution patterns leading to best ChC inhibitors (both for carboxylates as well as for the hydroxamates) were those involving perfluoroalkylsulfonyl- and substituted arylsulfonyl moieties, such as C₆F₅SO₂, protected 3- and 4-aminophenylsulfonyl-, 3-/4-HO₂CC₆H₄SO₂, 3-F₃CC₆H₄SO₂, as well as 1- and 2-naphthyl-, quinolin-8-yl- or substituted-arylsulfonylamido-carboxyl moieties among others. Similarly to the matrix metalloproteinase (MMP) hydroxamate inhibitors, ChC inhibitors of the type reported here must incorporate hydrophobic moieties at the P2' and P3' sites, to achieve tight binding to the enzyme. This study also proves that the 2-chlorobenzyl moiety, is an efficient P2' anchoring moiety for obtaining potent ChC inhibitors.

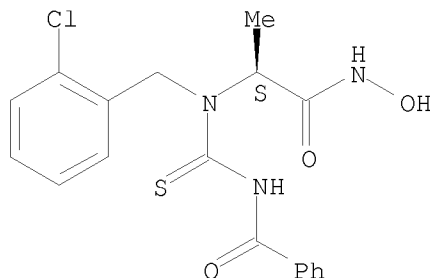
IT 269747-23-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of Clostridium collagenase inhibitors incorporating sulfonylated alanine hydroxamate)

RN 269747-23-1 HCAPLUS

CN Benzamide, N-[[[(2-chlorophenyl)methyl][(1S)-2-(hydroxyamino)-1-methyl-2-oxoethyl]amino]thioxomethyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

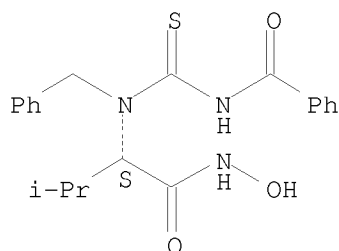
L37 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:142412 HCAPLUS

Updated Search

stn

DOCUMENT NUMBER: 132:342787
TITLE: Protease inhibitors. Part 7 Inhibition of Clostridium histolyticum collagenase with sulfonylated derivatives of l-valine hydroxamate
AUTHOR(S): Supuran, C. T.; Scozzafava, A.
CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy
SOURCE: European Journal of Pharmaceutical Sciences (2000), 10(1), 67-76
CODEN: EPSCED; ISSN: 0928-0987
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sulfonylated l-valine hydroxamate derivs. were obtained by reaction of alkyl/arylsulfonyl halides with the title amino acid, followed by treatment with benzyl chloride, and conversion of the COOH moiety to the CONHOH group. Other derivs. were obtained by reaction of N-benzyl-l-valine with arylisocyanates, arylsulfonylisocyanates or benzoylisothiocyanate, followed by the similar conversion of the COOH into the CONHOH moiety, with hydroxylamine in the presence of carbodiimides. The obtained compds. were assayed as inhibitors of the Clostridium histolyticum collagenase, ChC (EC 3.4.24.3), a zinc enzyme which degrades triple helical collagen. The hydroxamate derivs. were generally 100-500 times more active than the corresponding carboxylates. In the series of synthesized derivs., substitution patterns leading to best ChC inhibitors were those involving perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl; 3- and 4-protected-aminophenylsulfonyl-; 3- and 4-carboxyphenylsulfonyl-; 3-trifluoromethylphenylsulfonyl; or 1- and 2-naphthyl among others. Similarly to the matrix metalloproteinase hydroxamate inhibitors, ChC inhibitors of the type reported here must incorporate hydrophobic moieties at the P2' and P3' subsites, in order to achieve tight binding to the enzyme. Such compds. might lead to drugs useful in the treatment of corneal bacterial keratitis.
IT 270072-93-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonylated valine hydroxamates as inhibitors of Clostridium histolyticum collagenase)
RN 270072-93-0 HCAPLUS
CN Benzamide, N-[[[(1S)-1-[(hydroxyamino)carbonyl]-2-methylpropyl](phenylmethyl)amino]thioxomethyl]- (CA INDEX NAME)

Absolute stereochemistry.



Updated Search

stn

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3

L5 1 S L4 AND LIM, Z?/AU

L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED

L17 3 S L16

L18 69 S L16 FULL

L19 69 S L18 NOT L3

L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008

L23 STRUCTURE UPLOADED

L24 0 S L23

L25 18 S L23 FULL

L26 18 S L25 NOT L13

L27 18 S L25 NOT L3

L28 18 S L27 NOT L18

Updated Search

stn

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008

L29 1 S L28
L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008

L31 STRUCTURE UPLOADED
L32 1 S L31
L33 23 S L31 FULL
L34 23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008

L35 12 S L34
L36 11 S L35 NOT L14
L37 9 S L36 NOT L4
L38 0 S L37 AND LIM, Z?/AU
L39 0 S L37 AND WANG, H?/AU
L40 0 S L37 AND ZHOU, Y?/AU

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	75.95	1017.01
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.20	-11.20

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/CAplus. To learn more about the options available for

Updated Search

stn

transferring saved search queries and answer sets to CA/Caplus,
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=> s 134

L41 0 L34

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST	0.46	1017.47
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE	0.00	-11.20
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FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008

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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\asdfjafd.str

L42 STRUCTURE UPLOADED

=> s 142

SAMPLE SEARCH INITIATED 00:55:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 608 TO 1472

Updated Search

stn

PROJECTED ANSWERS: 1 TO 80

L43 1 SEA SSS SAM L42

=> s l42 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 00:55:29 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1051 TO ITERATE

100.0% PROCESSED 1051 ITERATIONS

74 ANSWERS

SEARCH TIME: 00.00.01

L44 74 SEA SSS FUL L42

=> dhis

DHIS IS NOT A RECOGNIZED COMMAND

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"HELP COMMANDS" at an arrow prompt (=>).

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3

L5 1 S L4 AND LIM, Z?/AU

L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED

L17 3 S L16

L18 69 S L16 FULL

Updated Search

stn

L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23 STRUCTURE UPLOADED
L24 0 S L23
L25 18 S L23 FULL
L26 18 S L25 NOT L13
L27 18 S L25 NOT L3
L28 18 S L27 NOT L18

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L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31 STRUCTURE UPLOADED
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L33 23 S L31 FULL
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FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35 12 S L34
L36 11 S L35 NOT L14
L37 9 S L36 NOT L4
L38 0 S L37 AND LIM, Z?/AU
L39 0 S L37 AND WANG, H?/AU
L40 0 S L37 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41 0 S L34

FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42 STRUCTURE UPLOADED
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L45 74 L44 NOT L34

=> s l45 not l19
L46 74 L45 NOT L19

=> d his

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Updated Search

stn

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FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

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L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

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FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

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FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

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FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED

L17 3 S L16

L18 69 S L16 FULL

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L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

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FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008

L23 STRUCTURE UPLOADED

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FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008

L29 1 S L28

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FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008

L31 STRUCTURE UPLOADED

L32 1 S L31

L33 23 S L31 FULL

L34 23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008

Updated Search

stn

L35 12 S L34
L36 11 S L35 NOT L14
L37 9 S L36 NOT L4
L38 0 S L37 AND LIM, Z?/AU
L39 0 S L37 AND WANG, H?/AU
L40 0 S L37 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
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FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
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L44 74 S L42 FULL
L45 74 S L44 NOT L34
L46 74 S L45 NOT L19

=> s l46 not l13
L47 74 L46 NOT L13

=> file hcaplus		
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	ENTRY	SESSION
FULL ESTIMATED COST	179.74	1197.21
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-11.20

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s 147

L48 13 L47

=> d hsi

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ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
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CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
 SCAN must be entered on the same line as the DISPLAY,
 e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, CLASS

IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
 containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
 its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
 its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs

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ENTER DISPLAY FORMAT (BIB):end

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(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

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L18 69 S L16 FULL
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FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

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FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

L22 0 S L20

Updated Search

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FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008

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FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008

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L33 23 S L31 FULL
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L37 9 S L36 NOT L4
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FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008

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=> d his

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L6 2 S L4 NOT L5

Updated Search

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L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
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FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
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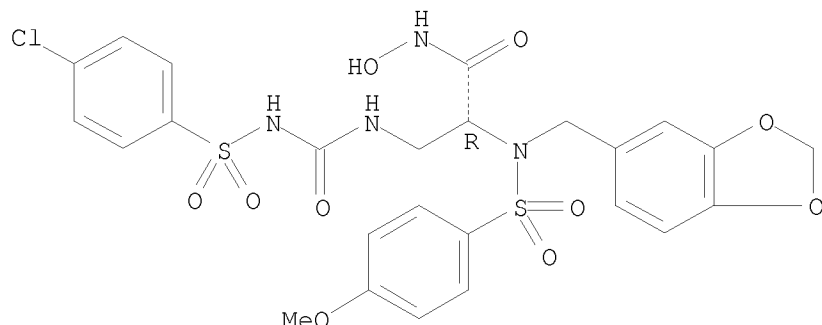
L49 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:442742 HCAPLUS
DOCUMENT NUMBER: 139:245665
TITLE: Novel Inhibitors of Procollagen C-Terminal Proteinase.
Part 1: Diamino Acid Hydroxamates
AUTHOR(S): Delaet, N. G. J.; Robinson, L. A.; Wilson, D. M.;
Sullivan, R. W.; Bradley, E. K.; Dankwardt, S. M.;
Martin, R. L.; Van Wart, H. E.; Walker, K. A. M.
CORPORATE SOURCE: CombiChem Inc., San Diego, CA, 92121, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003),
13(13), 2101-2104
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245665
AB The parallel synthesis of novel inhibitors of procollagen C-terminal
proteinase is described. The synthetic strategy allowed for the facile
synthesis of a large number of side-chain diversified diamino acid
hydroxamates, of which the d-diaminopropionic acid derivs. were shown to
be single digit nanomolar PCP inhibitors.
IT 279255-40-2P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(solid-phase synthesis and structure-activity relations of diamino acid
hydroxamates as inhibitors of procollagen C-terminal proteinase)
RN 279255-40-2 HCAPLUS
CN Propanamide, 2-[(1,3-benzodioxol-5-ylmethyl)[(4-
methoxyphenyl)sulfonyl]amino]-3-[[[(4-
chlorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy-, (2R)- (CA INDEX

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NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:311217 HCAPLUS

DOCUMENT NUMBER: 139:245734

TITLE: Protease inhibitors: synthesis of bacterial collagenase and matrix metalloproteinase inhibitors incorporating arylsulfonylureido and 5-dibenzo-suberenyl/suberyl moieties

AUTHOR(S): Ilies, Monica; Banciu, Mircea D.; Scozzafava, Andrea; Ilies, Marc A.; Caproiu, Miron T.; Supuran, Claudiu T.
CORPORATE SOURCE: Polo Scientifico, Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, 50019, Italy

SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(10), 2227-2239

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:245734

AB Novel matrix metalloproteinase (MMP)/bacterial collagenase inhibitors are reported, considering the sulfonylated amino acid hydroxamates as lead mols. A series of compds. was prepared by reaction of arylsulfonyl isocyanates with N-(5H-dibenzo[a,d]cyclohepten-5-yl)- and N-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl) Me glycolate, resp., followed by the conversion of the COOMe to the carboxylate/hydroxamate moieties. The corresponding derivs. with methylene and ethylene spacers between the polycyclic moiety and the amino acid functionality were also obtained by related synthetic strategies. These new compds. were assayed as inhibitors of MMP-1, MMP-2, MMP-8 and MMP-9, and of the collagenase isolated from *Clostridium histolyticum* (ChC). Some of the new derivs. reported here proved to be powerful inhibitors of the four MMPs mentioned above and of ChC, with activities in the low nanomolar range for some of the target enzymes, depending on the substitution pattern at the sulfonylureido moiety and on the length of the spacer through which the dibenzosuberenyl/suberyl group is connected with the rest of the mol.

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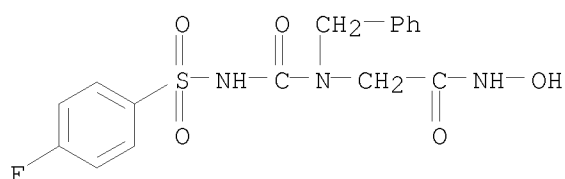
Several of these inhibitors also showed selectivity for the deep pocket enzymes (MMP-2, MMP-8 and MMP-9) over the shallow pocket ones MMP-1 and ChC.

IT 276695-94-4 276695-95-5 276695-96-6
276695-97-7

RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of arylsulfonylureido- and dibenzosuberonyl/suberyl-containing
compds. as matrix metalloproteinase/bacterial collagenase inhibitors)

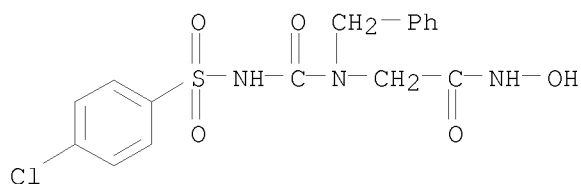
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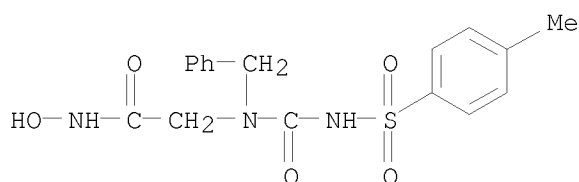
RN 276695-95-5 HCAPLUS

CN Acetamide, 2-[[[(4-chlorophenyl)sulfonyl]amino]carbonyl](phenylmethyl)amino]-N-hydroxy- (CA INDEX NAME)



RN 276695-96-6 HCAPLUS

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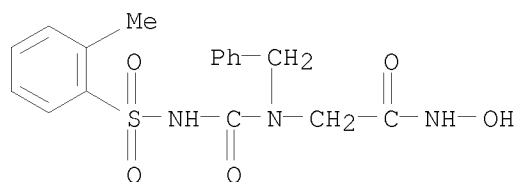


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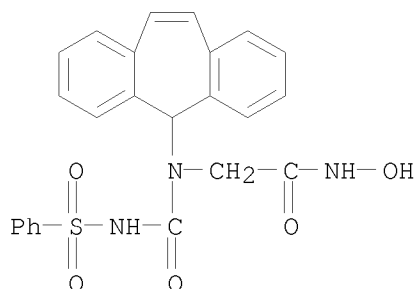
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 597570-47-3P 597570-49-5P 597570-51-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)

(preparation of arylsulfonylureido- and dibenzosuberonyl/suberyl-containing
 compds. as matrix metalloproteinase/bacterial collagenase inhibitors)

RN 597570-12-2 HCAPLUS

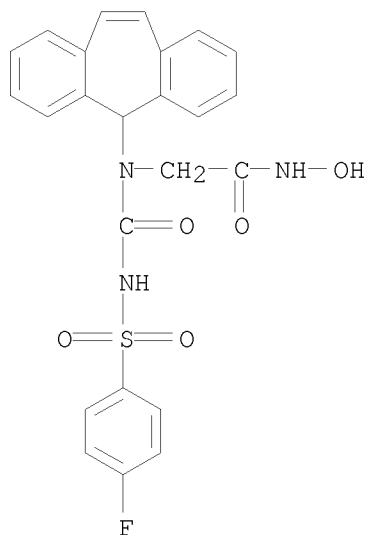
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RN 597570-13-3 HCAPLUS

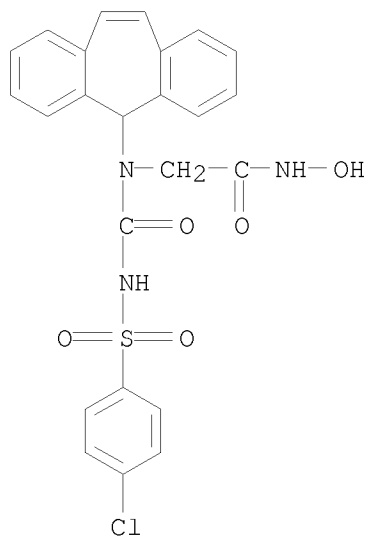
CN Acetamide, 2-[5H-dibenzo[a,d]cyclohepten-5-yl[[[(4-fluorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

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RN 597570-14-4 HCAPLUS

CN Acetamide, 2-[[[[(4-chlorophenyl)sulfonyl]amino]carbonyl]-5H-dibenzo[a,d]cyclohepten-5-ylamino]-N-hydroxy- (CA INDEX NAME)

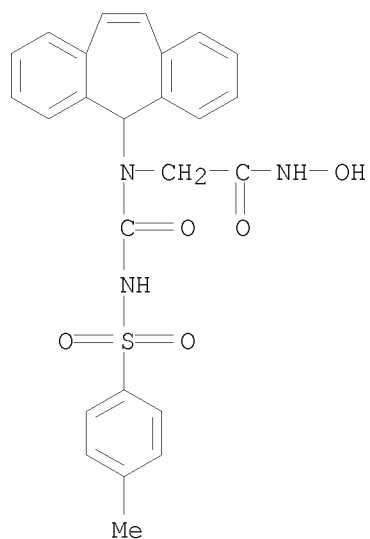


RN 597570-15-5 HCAPLUS

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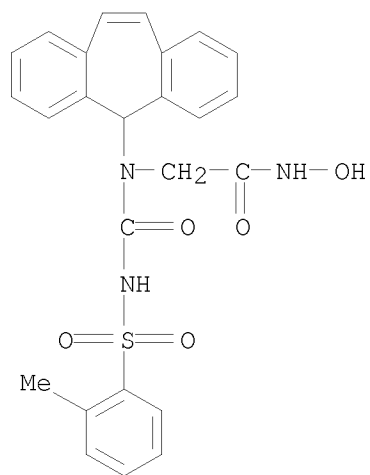
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RN 597570-16-6 HCAPLUS

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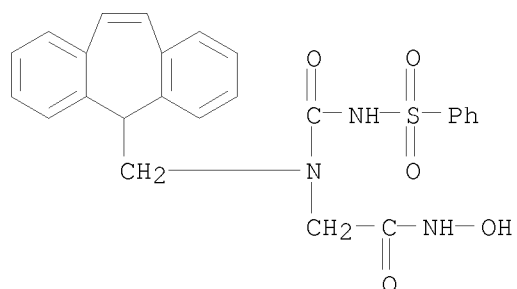


RN 597570-17-7 HCAPLUS

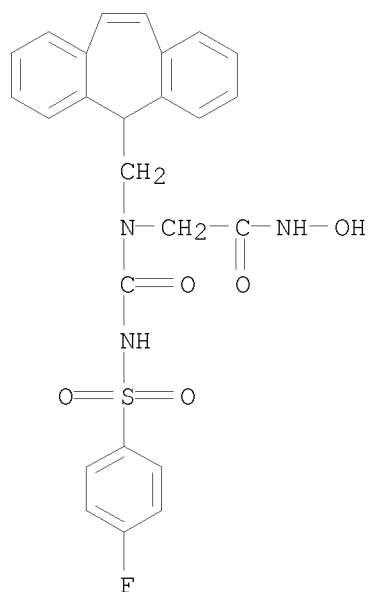
CN Acetamide, 2-[(5H-dibenzo[a,d]cyclohepten-5-ylmethyl)[[(phenylsulfonyl)amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

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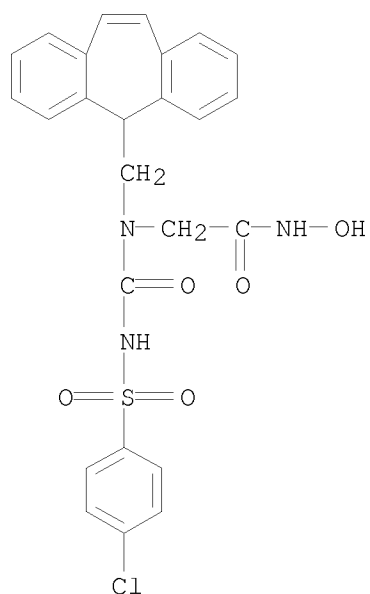
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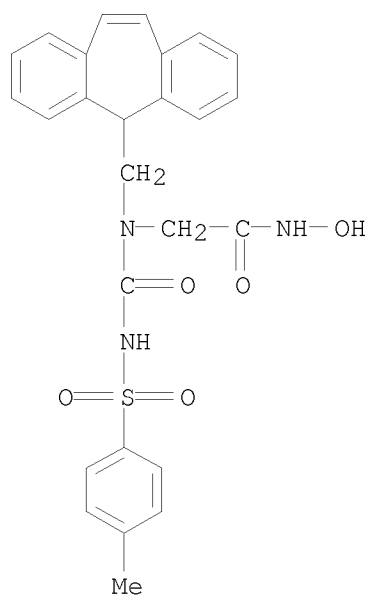
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 CN Acetamide, 2-[[[[(4-chlorophenyl)sulfonyl]amino]carbonyl] (5H-dibenzo[a,d]cyclohepten-5-ylmethyl)amino]-N-hydroxy- (CA INDEX NAME)

Updated Search

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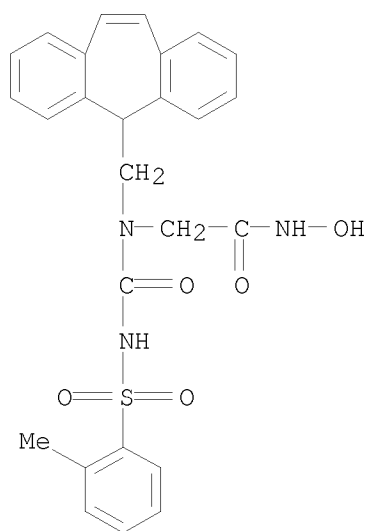
RN 597570-20-2 HCAPLUS
CN Acetamide, 2-[(5H-dibenzo[a,d]cyclohepten-5-ylmethyl) [[[4-methylphenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)



RN 597570-21-3 HCAPLUS
CN Acetamide, 2-[(5H-dibenzo[a,d]cyclohepten-5-ylmethyl) [[[2-methylphenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

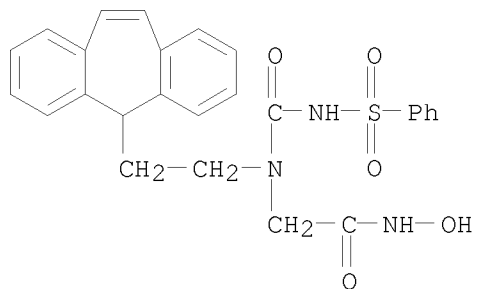
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RN 597570-22-4 HCAPLUS

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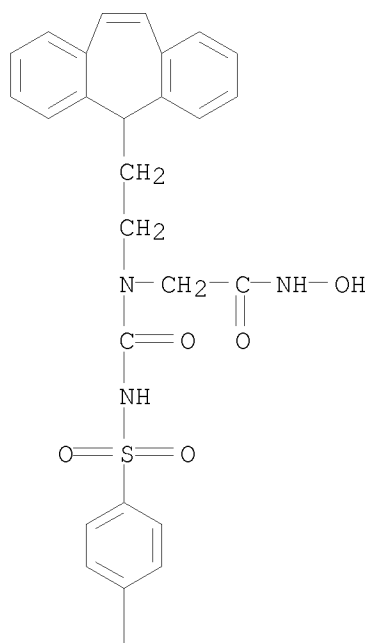
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CN Acetamide, 2-[[2-(5H-dibenzo[a,d]cyclohepten-5-yl)ethyl][[(4-fluorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

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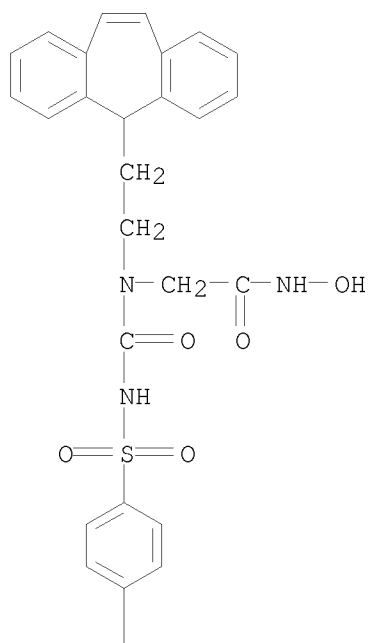
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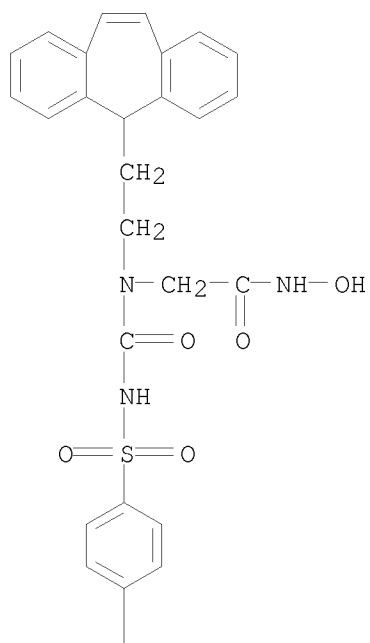
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PAGE 1-A



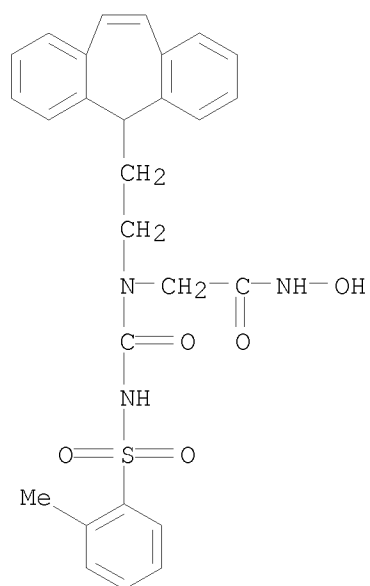
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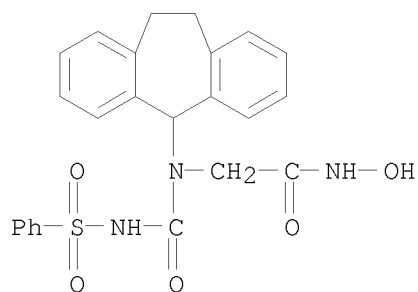
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CN Acetamide, 2-[[2-(5H-dibenzo[a,d]cyclohepten-5-yl)ethyl] [[[2-methylphenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

Updated Search

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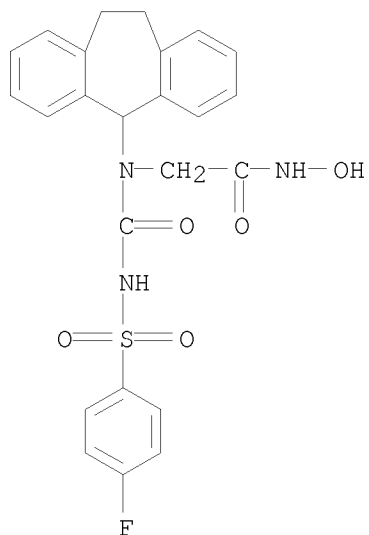
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RN 597570-28-0 HCAPLUS
 CN Acetamide, 2-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl) [[[4-(fluorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

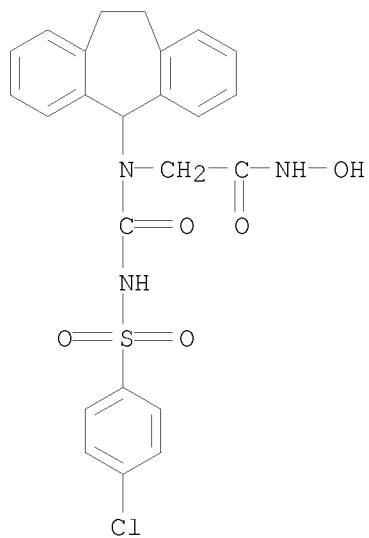
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RN 597570-29-1 HCAPLUS

CN Acetamide, 2-[[[[(4-chlorophenyl)sulfonyl]amino]carbonyl](10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)amino]-N-hydroxy- (CA INDEX NAME)

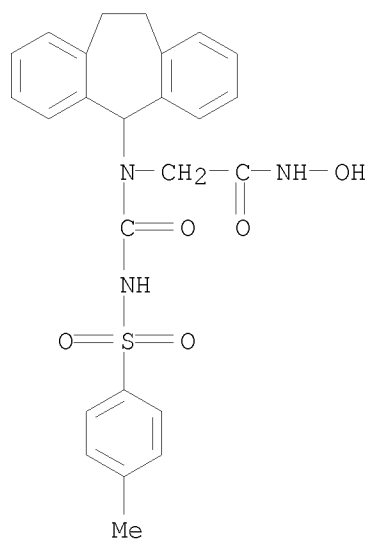


RN 597570-30-4 HCAPLUS

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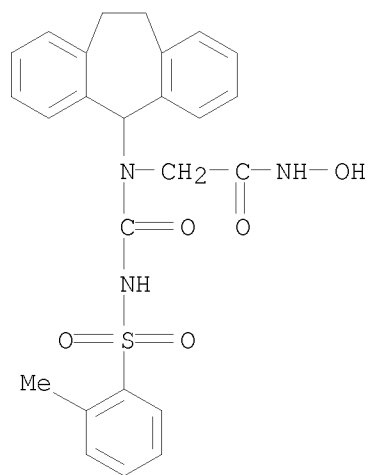
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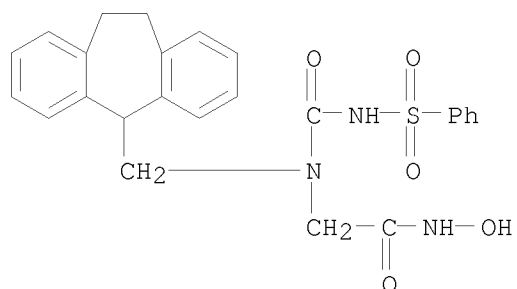


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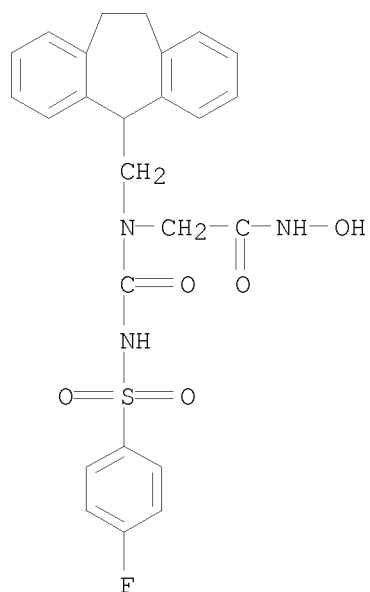
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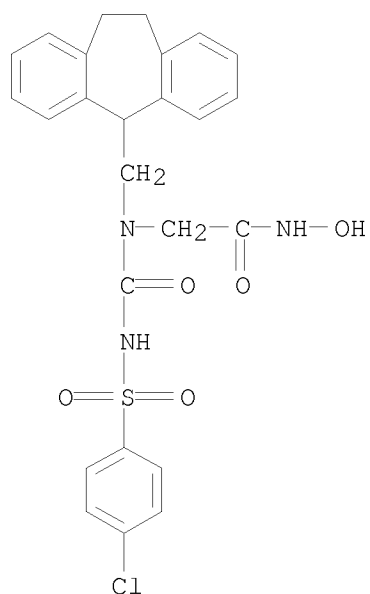


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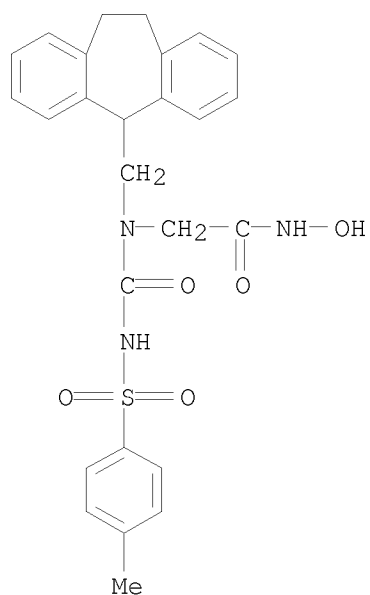
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RN 597570-39-3 HCAPLUS

CN Acetamide, 2-[[[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)methyl][[(4-methylphenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

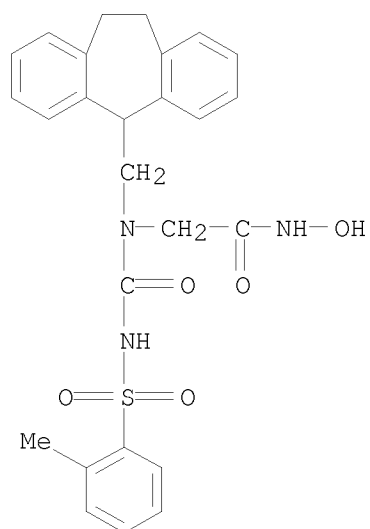


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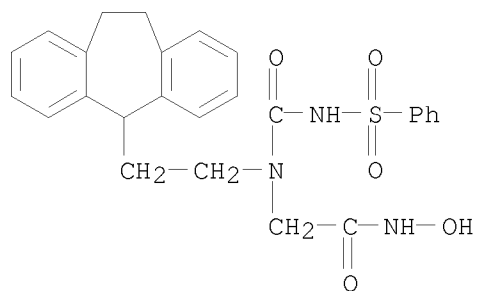
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Updated Search

stn



RN 597570-43-9 HCAPLUS
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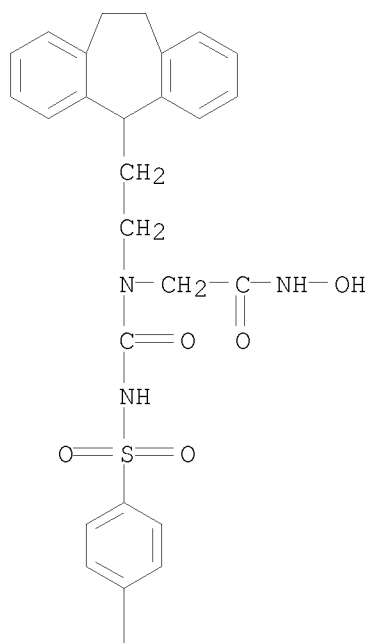


RN 597570-45-1 HCAPLUS
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Updated Search

stn

PAGE 1-A



PAGE 2-A

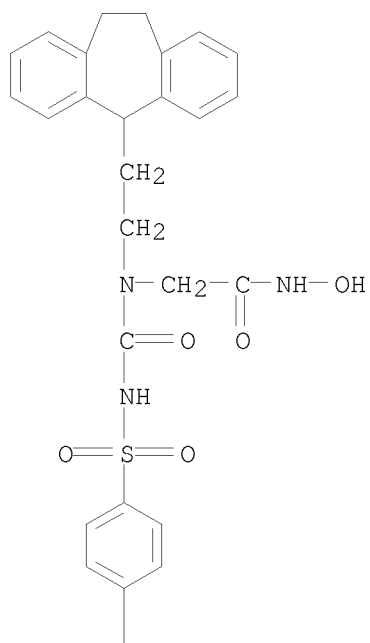
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RN 597570-47-3 HCAPLUS
CN Acetamide, 2-[[[[(4-chlorophenyl)sulfonyl]amino]carbonyl][2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)ethyl]amino]-N-hydroxy- (CA INDEX NAME)

Updated Search

stn

PAGE 1-A



PAGE 2-A

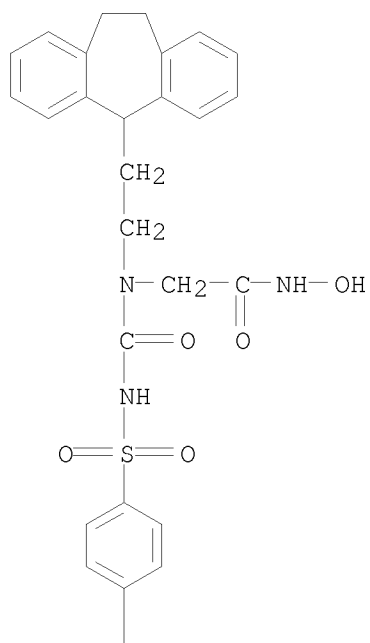
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RN 597570-49-5 HCAPLUS
CN Acetamide, 2-[[2-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)ethyl]N-[(4-methylphenyl)sulfonyl]carbamoyl]acetamido]-N-hydroxy- (CA INDEX NAME)

Updated Search

stn

PAGE 1-A



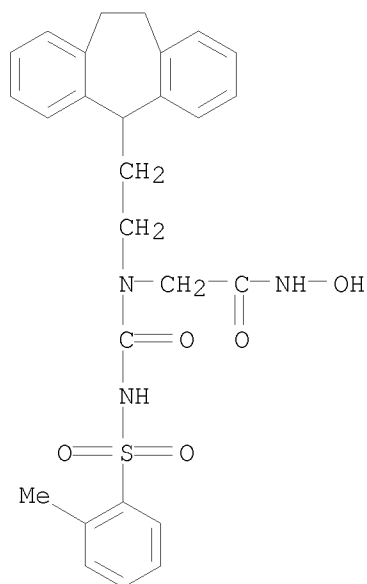
PAGE 2-A

Me

RN 597570-51-9 HCAPLUS
CN Acetamide, 2-[[2-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)ethyl]N-[(2-methylphenyl)sulfonyl]amino]acetyl]hydroxylamine (CA INDEX NAME)

Updated Search

stn



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:441768 HCAPLUS

DOCUMENT NUMBER: 133:74324

TITLE: Preparation of amino acid sulfonamide hydroxamates as inhibitors of procollagen C-proteinase.

INVENTOR(S): Billedeau, Roland Joseph; Broka, Chris Allen; Campbell, Jeffrey Allen; Chen, Jian Jeffrey; Dankwardt, Sharon Marie; Delaet, Nancy; Robinson, Leslie Ann; Walker, Keith Adrian Murray

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 133 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2000037436	A1	20000629	WO 1999-EP9920	19991214
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2355902	A1	20000629	CA 1999-2355902	19991214
BR 9916504	A	20010911	BR 1999-16504	19991214

Updated Search

stn

EP 1149072	A1	20011031	EP 1999-963530	19991214
EP 1149072	B1	20040630		
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TR 200101868	T2	20011121	TR 2001-1868	19991214
HU 2001004658	A2	20020629	HU 2001-4658	19991214
HU 2001004658	A3	20051228		
JP 2002533322	T	20021008	JP 2000-589508	19991214
AU 769319	B2	20040122	AU 2000-19792	19991214
NZ 512292	A	20040326	NZ 1999-512292	19991214
AT 270271	T	20040715	AT 1999-963530	19991214
RU 2232751	C2	20040720	RU 2001-119461	19991214
US 6492394	B1	20021210	US 1999-469660	19991222
HR 2001000443	A1	20020630	HR 2001-443	20010614
ZA 2001005014	A	20020919	ZA 2001-5014	20010619
MX 2001PA06328	A	20010910	MX 2001-PA6328	20010620
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NO 2001003100	A	20010821	NO 2001-3100	20010621
US 20030199520	A1	20031023	US 2002-267292	20021009
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US 20030216405	A1	20031120	US 2002-267727	20021009
US 6787559	B2	20040907		

PRIORITY APPLN. INFO.:

US 1998-113311P	P	19981222
US 1999-147053P	P	19990803
US 1999-164138P	P	19991108
WO 1999-EP9920	W	19991214
US 1999-469660	A3	19991222

OTHER SOURCE(S): MARPAT 133:74324

AB HOHNCOCHR1NRSO2Ar2 [R1 = alkyl, haloalkyl, heteroalkyl, cycloalkyl, aryl, aralkyl, aralkenyl, heteroaryl, heteroaralkyl, aminl, aryl, aralkyl, etc.; R = CHR2Ar1, CHR2CH:CHAr1; Ar2 = specified (substituted) Ph, naphthyl; R2 = H, alkyl; with provisos], were prepared Thus, N-hydroxy-2(R)-[(3,4-methylenedioxybenzyl)(4-methoxy-2,3,6-trimethylbenzenesulfonyl)amino]-3-methylbutyramide was prepared by solution phase synthesis from BOC-D-Val-OH. Title compds. inhibited procollagen C-proteinase with IC50 0.01-2 µM.

IT 279255-40-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid sulfonamide hydroxamates as inhibitors of procollagen C-proteinase)

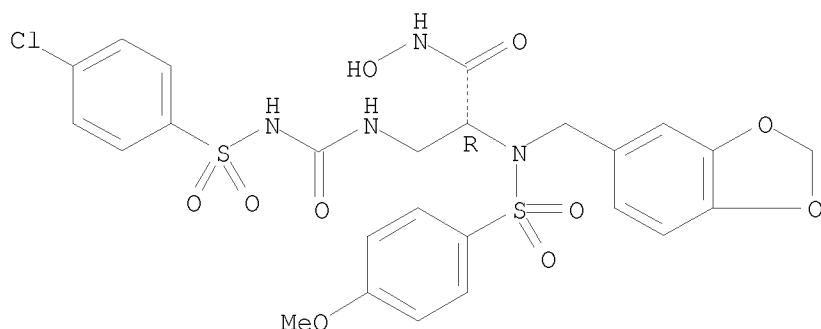
RN 279255-40-2 HCAPLUS

CN Propanamide, 2-[(1,3-benzodioxol-5-ylmethyl)[(4-methoxyphenyl)sulfonyl]amino]-3-[[[(4-chlorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

stn



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/CaPlus. To learn more about the options available for

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stn

transferring saved search queries and answer sets to CA/Caplus,
contact your STN Service Center.

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED
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L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008

L23 STRUCTURE UPLOADED
L24 0 S L23
L25 18 S L23 FULL
L26 18 S L25 NOT L13
L27 18 S L25 NOT L3
L28 18 S L27 NOT L18

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008

Updated Search

stn

L29 1 S L28
L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008

L31 STRUCTURE UPLOADED
L32 1 S L31
L33 23 S L31 FULL
L34 23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008

L35 12 S L34
L36 11 S L35 NOT L14
L37 9 S L36 NOT L4
L38 0 S L37 AND LIM, Z?/AU
L39 0 S L37 AND WANG, H?/AU
L40 0 S L37 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008

L41 0 S L34

FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008

L42 STRUCTURE UPLOADED
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L44 74 S L42 FULL
L45 74 S L44 NOT L34
L46 74 S L45 NOT L19
L47 74 S L46 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008

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L49 3 S L48 NOT L35
L50 0 S L49 AND LIM, Z?/AU
L51 0 S L49 AND WANG, H?/AU

FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008

=> s 147

L52 0 L47

=> file reg

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FULL ESTIMATED COST	0.46	1219.40
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CA SUBSCRIBER PRICE	0.00	-13.60

FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
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L53 STRUCTURE UPLOADED

=> s 153

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SAMPLE SCREEN SEARCH COMPLETED - 55 TO ITERATE

100.0% PROCESSED 55 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 656 TO 1544
PROJECTED ANSWERS: 0 TO 0

L54 0 SEA SSS SAM L53

=> s 153 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED - 1172 TO ITERATE

100.0% PROCESSED 1172 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L55 7 SEA SSS FUL L53

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

Updated Search

stn

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FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4          3 S L3
L5          1 S L4 AND LIM, Z?/AU
L6          2 S L4 NOT L5
L7          0 S L6 AND WANG, H?/AU
L8          0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9          0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
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L11         3 S L10
L12         66 S L10 FULL
L13         66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14         1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15         0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16         STRUCTURE UPLOADED
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L18         69 S L16 FULL
L19         69 S L18 NOT L3
L20         3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21         1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22         0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23         STRUCTURE UPLOADED
L24         0 S L23
L25         18 S L23 FULL
L26         18 S L25 NOT L13
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L28         18 S L27 NOT L18

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29         1 S L28
L30         0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31         STRUCTURE UPLOADED
L32         1 S L31
L33         23 S L31 FULL
L34         23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35         12 S L34
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Updated Search

stn

L36 11 S L35 NOT L14
L37 9 S L36 NOT L4
L38 0 S L37 AND LIM, Z?/AU
L39 0 S L37 AND WANG, H?/AU
L40 0 S L37 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008

L41 0 S L34

FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008

L42 STRUCTURE UPLOADED
L43 1 S L42
L44 74 S L42 FULL
L45 74 S L44 NOT L34
L46 74 S L45 NOT L19
L47 74 S L46 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008

L48 13 S L47
L49 3 S L48 NOT L35
L50 0 S L49 AND LIM, Z?/AU
L51 0 S L49 AND WANG, H?/AU

FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008

L52 0 S L47

FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008

L53 STRUCTURE UPLOADED
L54 0 S L53
L55 7 S L53 FULL

=> s l55 not l47

L56 7 L55 NOT L47

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	0.00	-13.60

FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008

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Updated Search

stn

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l56

L57 1 L56

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

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L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

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L5 1 S L4 AND LIM, Z?/AU

L6 2 S L4 NOT L5

L7 0 S L6 AND WANG, H?/AU

L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED

L17 3 S L16

L18 69 S L16 FULL

L19 69 S L18 NOT L3

L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

Updated Search

stn

L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008

L23 STRUCTURE UPLOADED

L24 0 S L23

L25 18 S L23 FULL

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L29 1 S L28

L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008

L31 STRUCTURE UPLOADED

L32 1 S L31

L33 23 S L31 FULL

L34 23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008

L35 12 S L34

L36 11 S L35 NOT L14

L37 9 S L36 NOT L4

L38 0 S L37 AND LIM, Z?/AU

L39 0 S L37 AND WANG, H?/AU

L40 0 S L37 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008

L41 0 S L34

FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008

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L43 1 S L42

L44 74 S L42 FULL

L45 74 S L44 NOT L34

L46 74 S L45 NOT L19

L47 74 S L46 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008

L48 13 S L47

L49 3 S L48 NOT L35

L50 0 S L49 AND LIM, Z?/AU

L51 0 S L49 AND WANG, H?/AU

FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008

L52 0 S L47

FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008

L53 STRUCTURE UPLOADED

L54 0 S L53

L55 7 S L53 FULL

L56 7 S L55 NOT L47

Updated Search

stn

FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
L57 1 S L56

=> s 157 not 129
L58 0 L57 NOT L29

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.69	1401.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-13.60

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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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experimental property data in the original document. For information
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\sadfaerat.str

L59 STRUCTURE UPLOADED

=> s 159
SAMPLE SEARCH INITIATED 01:00:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

Updated Search

stn

PROJECTED ITERATIONS: 608 TO 1472
PROJECTED ANSWERS: 0 TO 0

L60 0 SEA SSS SAM L59

=> s l59 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED - 1051 TO ITERATE

100.0% PROCESSED 1051 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L61 2 SEA SSS FUL L59

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008

L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008

L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008

L21 1 S L20

Updated Search

stn

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FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22      0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23      STRUCTURE UPLOADED
L24      0 S L23
L25      18 S L23 FULL
L26      18 S L25 NOT L13
L27      18 S L25 NOT L3
L28      18 S L27 NOT L18

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29      1 S L28
L30      0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31      STRUCTURE UPLOADED
L32      1 S L31
L33      23 S L31 FULL
L34      23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35      12 S L34
L36      11 S L35 NOT L14
L37      9 S L36 NOT L4
L38      0 S L37 AND LIM, Z?/AU
L39      0 S L37 AND WANG, H?/AU
L40      0 S L37 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41      0 S L34

FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42      STRUCTURE UPLOADED
L43      1 S L42
L44      74 S L42 FULL
L45      74 S L44 NOT L34
L46      74 S L45 NOT L19
L47      74 S L46 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48      13 S L47
L49      3 S L48 NOT L35
L50      0 S L49 AND LIM, Z?/AU
L51      0 S L49 AND WANG, H?/AU

FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52      0 S L47

FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53      STRUCTURE UPLOADED
L54      0 S L53
L55      7 S L53 FULL
L56      7 S L55 NOT L47
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Updated Search

stn

FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008

L57 1 S L56
L58 0 S L57 NOT L29

FILE 'REGISTRY' ENTERED AT 00:59:15 ON 27 OCT 2008

L59 STRUCTURE UPLOADED
L60 0 S L59
L61 2 S L59 FULL

=> s 161 not 157
L62 0 L61 NOT L57

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\araty.str

L63 STRUCTURE UPLOADED

=> s 163
SAMPLE SEARCH INITIATED 01:02:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 65 TO ITERATE

100.0% PROCESSED 65 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 817 TO 1783
PROJECTED ANSWERS: 0 TO 0

L64 0 SEA SSS SAM L63

=> s 163 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 01:02:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1581 TO ITERATE

100.0% PROCESSED 1581 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L65 2 SEA SSS FUL L63

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008

L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5

Updated Search

stn

L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23 STRUCTURE UPLOADED
L24 0 S L23
L25 18 S L23 FULL
L26 18 S L25 NOT L13
L27 18 S L25 NOT L3
L28 18 S L27 NOT L18

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29 1 S L28
L30 0 S L29 NOT L21

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31 STRUCTURE UPLOADED
L32 1 S L31
L33 23 S L31 FULL
L34 23 S L33 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35 12 S L34
L36 11 S L35 NOT L14
L37 9 S L36 NOT L4
L38 0 S L37 AND LIM, Z?/AU
L39 0 S L37 AND WANG, H?/AU
L40 0 S L37 AND ZHOU, Y?/AU

Updated Search

stn

FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41 0 S L34

FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42 STRUCTURE UPLOADED
L43 1 S L42
L44 74 S L42 FULL
L45 74 S L44 NOT L34
L46 74 S L45 NOT L19
L47 74 S L46 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48 13 S L47
L49 3 S L48 NOT L35
L50 0 S L49 AND LIM, Z?/AU
L51 0 S L49 AND WANG, H?/AU

FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52 0 S L47

FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53 STRUCTURE UPLOADED
L54 0 S L53
L55 7 S L53 FULL
L56 7 S L55 NOT L47

FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
L57 1 S L56
L58 0 S L57 NOT L29

FILE 'REGISTRY' ENTERED AT 00:59:15 ON 27 OCT 2008
L59 STRUCTURE UPLOADED
L60 0 S L59
L61 2 S L59 FULL
L62 0 S L61 NOT L57
L63 STRUCTURE UPLOADED
L64 0 S L63
L65 2 S L63 FULL

=> s l65 not l56
L66 2 L65 NOT L56

=> file hcaplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	358.10	1759.47
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-13.60

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l65

L67 1 L65

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

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FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008

L10 STRUCTURE UPLOADED

L11 3 S L10

L12 66 S L10 FULL

L13 66 S L12 NOT L3

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L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

L15 0 S L13

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FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
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L27 18 S L25 NOT L3
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L33 23 S L31 FULL
L34 23 S L33 NOT L13

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L48 13 S L47
L49 3 S L48 NOT L35
L50 0 S L49 AND LIM, Z?/AU
L51 0 S L49 AND WANG, H?/AU

Updated Search

stn

```
FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52      0 S L47

FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53      STRUCTURE UPLOADED
L54      0 S L53
L55      7 S L53 FULL
L56      7 S L55 NOT L47

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L60      0 S L59
L61      2 S L59 FULL
L62      0 S L61 NOT L57
L63      STRUCTURE UPLOADED
L64      0 S L63
L65      2 S L63 FULL
L66      2 S L65 NOT L56

FILE 'HCAPLUS' ENTERED AT 01:02:29 ON 27 OCT 2008
L67      1 S L65

=> s 167 not 157
L68      0 L67 NOT L57
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Updated Search